

Complete decomposition of 1-chloropropane behind the reflected Shock Waves in the temperature range of 950 - 1480K

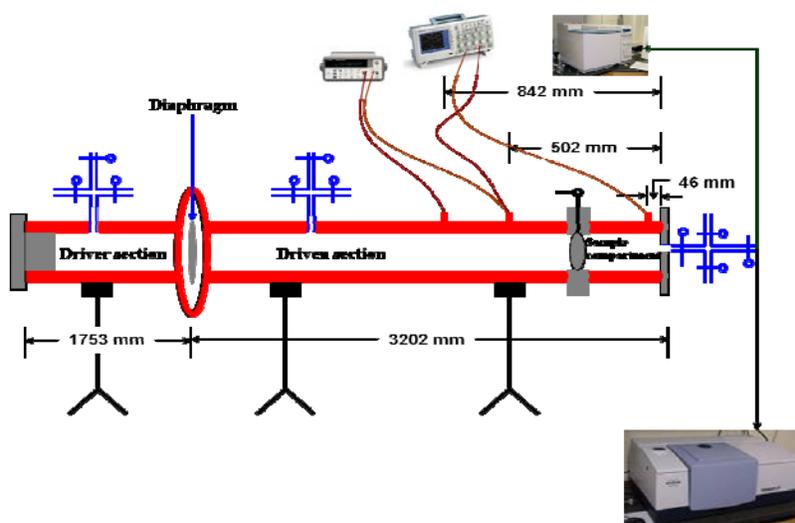
G. Sudhakar,¹ B. Rajakumar,^{1,*}

¹ Indian Institute of Technology Madras, Chennai 600 036, INDIA

A Single Pulse Shock Tube (SPST) facility is built and calibrated in our research laboratory at IIT Madras to study the kinetics and thermo chemistry of various molecules of interest in combustion as well as in Earth's atmosphere. Using this facility, thermal decomposition of 1-chloropropane was investigated in the temperature range of 950 - 1480K behind the single pulse reflected shock waves. The decomposition was carried out at a relative pressure of 25 bar with a typical reaction times of 500 μ s. Unimolecular elimination of HCl was found to be the major decomposition channel when the temperatures are below 1150K, which was in consistent with the earlier studies^{1,2}. The C-C bond dissociation becomes dominant at higher temperatures and leads to the formation of various products. While propylene, Ethylene being major products, methane, ethane and propane were observed to be minor products. The rate coefficients for the major as well as minor channels are obtained in the present study. The complete decomposition is simulated with the most appropriate reaction mechanism in the covered temperature range. In addition to the experimental studies, DFT calculations have been carried out to find the major decomposition pathways and compared with the experimental results. The complete results will be discussed in the presentation at the conference.

References

- (1) Okada, K.; Tschuikow-Roux, E.; Evans, P.J. *J. Phys. Chem.* **1980**, 84, 467 – 471.
- (2) Evans, P.J.; Ichimura, T.; Tschuikow-Roux, E. *Int. J. Chem. Kinet.* **1978**, 10, 855 - 869.



Schematic diagram of the established SPST facility at IIT Madras